Quantum tunnelling of a complex system: effects of a finite size and intrinsic structure

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Abstract

A simple model is considered to study the effects of finite size and internal structure in the tunnelling of bound two-body systems through a potential barrier. It is demonstrated that these effects are able to increase the tunnelling probability. Applications may include nuclear fusion, hydrogen atom and Cooper pair tunnelling.

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I. INTRODUCTION

The processes using the mechanism of quantum tunnelling are abundant in different areas of physics. Chemical reactions at low temperatures, diverse phenomena in solid state physics, nuclear alpha and cluster decays, fission and fusion processes in thermonuclear reactors, shortly after the Big Bang and inside stellar matter proceed through the Coulomb barrier. The conventional textbook treatment is, as a rule, limited by considering tunnelling of a point-like object. It is known that the intrinsic degrees of freedom of a system modelled by a barrier are important, and one needs to take into account the probabilistic distribution of barriers [1] in order to explain the subbarrier fusion. The friction-like processes under the barrier hinder the tunnelling [2]. At the same time, interaction of a charged particle with virtual electromagnetic field (an analog of the Lamb shift in bound states) increases the tunnelling probability [3]. In reality, in many cases one has to deal with the tunnelling of a composite object with its own intrinsic degrees of freedom.

An important question of how the tunnelling reactions are influenced by the finite size and the structure of the tunnelling object remains poorly understood. For example, the deuteron is a weakly bound complex with a size that is large on nuclear scale. How does this size influence the fusion reaction $d + d \rightarrow {}^4\text{He}$ deeply under the Coulomb barrier? There are no experimental laboratory data for the fusion cross section at low ($\sim$ keV) deuteron energies, since the cross section is too small. However, there is a discrepancy between the standard theory and the existing measurements for dd-reactions in solids at energy between 10 and 2 keV [4,5]. This is an area of extreme importance for astrophysical and thermonuclear applications, especially with the perspective of radioactive beam facilities of new generation. Currently, the nuclear cross sections for low energies are determined by extrapolation based on the results for point-like tunnelling particles.

Another example of great interest in relation to various tunnelling devices is given by electron Cooper pairs in superconductors. In "usual" superconductors, the size of the pair is so large that the electron binding is of minor significance for such processes, and the Josephson tunnelling matrix element can be taken as a product of penetrabilities for independent electrons. In high-temperature superconductors, the size of the pair is much smaller, and the binding may produce corrections. The tunneling of a bound electron pair through the potential barrier created at the "point contact" in semiconductors is also of interest because this process may be related to the mysterious $0.7(2e^2/\hbar)$ structure in the measurements of conductance quantization in one-dimensional systems [6] (note that a bound pair appears in a one-dimensional system even for an arbitrary weak attraction). One can also be interested in finite size effects for hydrogen tunnelling (a system of one heavy particle and one light particle).

To provide an analytical estimate of the finite size effect we use a simple model. A system consists of two particles bound by the oscillator potential. An additional parabolic potential of positive or negative sign acts on one of the particles. This model allows one to study the limiting cases and shows that the finite size of a tunnelling system may be very important. Similar results for a pair of particles bound in an infinite potential box, while one of the particles encounters a rectangular barrier, were found in the old paper by Zakhariev and Sokolov [7], with the conclusion that the effective barrier is modified which facilitates the penetration. We show also that the electrostatic polarizability of a composite particle

adiabatically approaching the Coulomb barrier increases the tunnelling probability.

II. TWO OSCILLATORS

A. Normal modes

We consider two particles interacting via the harmonic potential and moving in the external field that acts on one particle only. The Hamiltonian of such a system is

$$H = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + \frac{1}{2}k(x-y)^2 + \frac{1}{2}qx^2. \tag{1}$$

Here coordinates, x and y, and corresponding momenta, p_x and p_y, refer to a "proton" and "neutron", respectively; the potential $(1/2)k(x-y)^2$ describes the binding of the particles, and the potential $(1/2)qx^2$ acts on the "proton" only. The case of $q < 0$ models a Coulomb potential barrier for the "proton" in the process of the fusion of two "deuterons" into ^{4}He or fusion of the "deuteron" with any other nucleus.

The secular equation for normal modes reads

$$\omega^4 - \omega^2 \left(\frac{k}{\mu} + \frac{q}{m_x} \right) + \frac{kq}{m_x m_y} = 0, \tag{2}$$

where the reduced mass $\mu = m_x m_y/(m_x + m_y)$. The solution may be conveniently written in terms of the parameters of bare frequencies and the ratio of the masses,

$$\nu^2 = \frac{k}{\mu}, \quad \Omega^2 = \frac{q}{m_x}, \quad \lambda = \frac{m_x}{m_x + m_y}. \tag{3}$$

Then the frequencies of two normal modes are

$$\omega_\pm^2 = \frac{1}{2}\left[\nu^2 + \Omega^2 \pm \sqrt{\nu^4 + \Omega^4 + 2\nu^2\Omega^2(1 - 2\lambda)} \right]; \tag{4}$$

at $q < 0$, ω_- is imaginary. The case of equal masses, $m_x = m_y = m$, is $\lambda = 1/2$, when

$$\omega_\pm^2 = \frac{1}{2}\left[\nu^2 + \Omega^2 \pm \sqrt{\nu^4 + \Omega^4} \right] = \frac{1}{2m}\left[q + 2k \pm \sqrt{q^2 + 4k^2} \right]. \tag{5}$$

If the x-particle ("proton") is very light, $m_x \to 0$, $\lambda \to 0$,

$$\omega_+^2 = \nu^2 + \Omega^2, \quad \omega_-^2 \to 0; \tag{6}$$

if the y-particle ("neutron") is very light, $m_x \to 0$, $\lambda \to 1$, two bare frequencies are normal modes,

$$\omega_+^2 = \nu^2, \quad \omega_-^2 = \Omega^2. \tag{7}$$

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B. Wave function

To find the spatial structure of the normal modes, we carry out the standard diagonalization of the Hamiltonian. First we make the scale transformation to new coordinates $u_{x,y}$ and new momenta $v_{x,y}$,

$$p_x = \sqrt{m_x}\, v_x, \quad p_y = \sqrt{m_y}\, v_y, \quad x = \frac{u_x}{\sqrt{m_x}}, \quad y = \frac{u_y}{\sqrt{m_y}}. \tag{8}$$

Then the Hamiltonian takes the form

$$H = \frac{1}{2}(v_x^2 + v_y^2) + \frac{k}{2}\left(\frac{u_x}{\sqrt{m_x}} - \frac{u_y}{\sqrt{m_y}}\right)^2 + \frac{1}{2}\frac{q u_x^2}{m_x}. \tag{9}$$

Since the kinetic form is invariant, we diagonalize the potential form by the orthogonal transformation

$$u_x = \xi_1 \cos\phi + \xi_2 \sin\phi, \quad u_y = -\xi_1 \sin\phi + \xi_2 \cos\phi. \tag{10}$$

The transformed potential energy is

$$U = \frac{1}{2}\xi_1^2 U_{11} + \frac{1}{2}\xi_2^2 U_{22} + \xi_1 \xi_2 U_{12}, \tag{11}$$

where

$$U_{11} = k\left(\frac{\cos\phi}{\sqrt{m_x}} + \frac{\sin\phi}{\sqrt{m_y}}\right)^2 + \frac{q}{m_x}\cos^2\phi, \tag{12}$$

$$U_{22} = k\left(\frac{\sin\phi}{\sqrt{m_x}} - \frac{\cos\phi}{\sqrt{m_y}}\right)^2 + \frac{q}{m_x}\sin^2\phi, \tag{13}$$

$$U_{12} = k\left(\frac{\cos\phi}{\sqrt{m_x}} + \frac{\sin\phi}{\sqrt{m_y}}\right)\left(\frac{\sin\phi}{\sqrt{m_x}} - \frac{\cos\phi}{\sqrt{m_y}}\right) + \frac{q}{m_x}\cos\phi\sin\phi. \tag{14}$$

The diagonalization condition $U_{12} = 0$ determines the mixing angle ϕ,

$$\tan(2\phi) = \frac{2k\sqrt{m_x m_y}}{qm_y + k(m_y - m_x)} = \frac{2\nu^2\sqrt{\lambda(1-\lambda)}}{\Omega^2 + \nu^2(1-2\lambda)}. \tag{15}$$

From here

$$\sin(2\phi) = \frac{2\nu^2\sqrt{\lambda(1-\lambda)}}{\sqrt{\Omega^4 + \nu^4 + 2\nu^2\Omega^2(1-2\lambda)}}, \tag{16}$$

$$\cos(2\phi) = \frac{\Omega^2 + \nu^2(1-2\lambda)}{\sqrt{\Omega^4 + \nu^4 + 2\nu^2\Omega^2(1-2\lambda)}}, \tag{17}$$

Therefore we get, as it should be, in agreement with (4),

$$U_{11} = \omega_+^2, \quad U_{22} = \omega_-^2. \tag{18}$$

The wave function of the system is the product of two oscillator functions,

$$\Psi(x,y) = \psi_1(\xi_1; \omega_+)\psi_2(\xi_2; \omega_-). \tag{19}$$

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III. PHYSICAL EFFECTS

A. Probability of tunnelling

The most interesting case corresponds to negative q and, whence, negative ω_-^2. The transmission coefficient for the parabolic barrier is given by [8]

$$T = \frac{D}{1+D},\tag{20}$$

where

$$D = \exp\left(\frac{2\pi E}{\hbar|\omega_-|}\right)\tag{21}$$

is the semiclassical penetrability for a "one-way" traverse. Here E is the energy of the "deuteron" for motion along the coordinate ξ_2, corresponding to the imaginary frequency; $E = 0$ corresponds to the top of the barrier. The tunnelling probability is exponentially small for $E < 0$. A realistic case corresponds to $k \gg |q|$, a "deuteron" bound much stronger than Coulomb energy. In this case (for equal masses)

$$|\omega_-| \approx \sqrt{\frac{|q|}{2m}}\left(1+\frac{|q|}{8k}\right) \equiv \omega_0\left(1+\frac{|q|}{8k}\right).\tag{22}$$

The factor $1 + |q|/(8k)$ provides an exponential enhancement of the tunnelling probability for the finite size "deuteron" in comparison with a particle of a zero size ($k = \infty$),

$$D = D_0 \exp\left(\frac{\pi|E|\sqrt{m|q|}}{2\sqrt{2}\hbar k}\right) = D_0 \exp\left(\frac{\pi|E|m\omega_0}{2\hbar k}\right),\tag{23}$$

where

$$D_0 = \exp\left(-\frac{2\pi|E|}{\hbar\omega_0}\right).\tag{24}$$

For the real deuteron this effect is too small but it increases if the "charged" particle is very light, $m_x/m_y \ll 1$,

$$|\omega_-| \approx \sqrt{\frac{|q|}{m_x+m_y}}\left(1+\frac{|q|}{8k}\frac{m_y}{m_x}\right).\tag{25}$$

B. Polarizability

There is another effect that may be even more important than the modification of the barrier (change of ω_-) considered in the preceding subsection and analogous to the effect of ref. [7]. This is energy transfer from internal motion of the "deuteron" to the translational

motion which happens for a non-parabolic barrier. Let us consider a more realistic model, where the potential barrier is smoothly goes to zero at infinity being parabolic near the top. The change of internal motion of the "deuteron" in the ground state occurs adiabatically as a transition from the unperturbed value $\hbar\nu/2$ far away from the barrier to $\hbar\omega_+/2$. This energy difference is converted into energy of translational motion of the "deuteron":

$$E = E(\infty) + \frac{\hbar\nu}{2} - \frac{\hbar\omega_+}{2} \approx E(\infty) + \frac{\hbar q}{4\sqrt{km_x}}\left(\frac{m_y}{m_x + m_y}\right)^{3/2}. \tag{26}$$

This correction also grows if the "charged" particle is light.

For the real deuteron (or any charged system) this correction may be presented as a result of the deuteron polarization,

$$E = E(\infty) + \frac{1}{2}\alpha\mathcal{E}^2, \tag{27}$$

where α is the deuteron polarizability and $\mathcal{E}$ the electric field produced by the Coulomb field. The internal ground state energy decreases by this amount, $\delta E = -\alpha\mathcal{E}^2/2$, that is transferred into translational motion. Indeed, the electric field polarizes the deuteron (the electric dipole moment is $d = \alpha\mathcal{E}$). This creates an additional force, $(d/dx)\alpha\mathcal{E}^2/2$. Integration of this force gives a positive correction to kinetic energy, or, to present it more conveniently, a negative correction to the Coulomb barrier potential,

$$\delta U = -\frac{1}{2}\alpha\mathcal{E}^2 = -\alpha\frac{Z^2 e^2}{2r^4}. \tag{28}$$

Again, this correction increases the barrier penetration factor. For the deuteron, the empirical value [9] is α=0.70(5) fm^3. We can estimate the change of the Coulomb barrier penetration factor due to this potential ($U = Ze^2/r + \delta U$). In the WKB semiclassical approximation,

$$D = \exp\left(-\frac{2\pi Z e^2}{\hbar v}\right)\exp\left(\frac{\alpha Z^{3/2} e\sqrt{2m}}{5\hbar(r_c)^{5/2}}\right), \tag{29}$$

where v is the relative velocity, m the reduced mass for two nuclei, and r_c the cut-off radius where the validity of the potential approximated by $U = Ze^2/r + \delta U$ is violated ($r_c \sim r_d$ where r_d is the deuteron radius). For the fusion of two deuterons, the correction due to the polarization potential is small ($\sim 1\%$). However, it rapidly increases with the nuclear charge.

C. "Cold fusion" and muon catalysis

In a process of muon catalysis, the fusion proceeds from a ground state of a muonic molecule, $dd\mu$ or $dt\mu$. This process occurs due to zero-point oscillations in the ground state of the molecule, as soon as a neutron from one nucleus reaches the strong potential well of another nucleus. In the two-oscillator model with $q > 0$, the expectation values of the normal coordinates in the ground states are

$$\langle \xi_1^2 \rangle = \frac{\hbar}{2\omega_+}, \quad \langle \xi_2^2 \rangle = \frac{\hbar}{2\omega_-}, \quad \langle \xi_1 \xi_2 \rangle = 0. \tag{30}$$

Going back to the original coordinates, eqs. (8) and (10), we find

$$\langle x^2 \rangle = \frac{\hbar}{2m_x} \left(\frac{\cos^2 \phi}{\omega_+} + \frac{\sin^2 \phi}{\omega_-} \right), \tag{31}$$

$$\langle y^2 \rangle = \frac{\hbar}{2m_y} \left(\frac{\cos^2 \phi}{\omega_-} + \frac{\sin^2 \phi}{\omega_+} \right), \tag{32}$$

$$\langle xy \rangle = \frac{\hbar \sin \phi \, \cos \phi}{2\sqrt{m_x m_y}} \left(\frac{1}{\omega_-} - \frac{1}{\omega_+} \right). \tag{33}$$

The oscillations of the "neutron" are described by $\langle y^2 \rangle$. In the most interesting case $k \gg q$ we have

$$\langle y^2 \rangle = \frac{\hbar}{2\sqrt{2mq}} \left(1 + \sqrt{\frac{q}{4k}} \right), \tag{34}$$

In this approximation the result for the "proton" oscillations $\langle x^2 \rangle$ is the same. Again, the finite size of the "deuteron" leads to stretching of the zero-point oscillations by a factor $(1 + \sqrt{q/4k})$ and to the enhancement of the fusion probability.

D. Tunnelling of a bound electron (Cooper) pair

The Hamiltonian of such a system may be modelled as

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}k(x - y)^2 + \frac{1}{2}q(x^2 + y^2). \tag{35}$$

Then the frequencies of two normal modes are

$$\omega_+^2 = \frac{2k + q}{m}, \quad \omega_-^2 = \frac{q}{m}. \tag{36}$$

At $q < 0$, ω_- is imaginary. It does not depend on k, therefore the parabolic barrier for center-of-mass motion is not modified by the finite size of the system. However, there is the energy transfer from the internal motion to the translational motion if the potential barrier smoothly goes to zero at large distances being parabolic near the top:

$$E = E(\infty) + \frac{\hbar\sqrt{2k/m}}{2} - \frac{\hbar\sqrt{(2k + q)/m}}{2}. \tag{37}$$

This energy transfer increases the tunnelling probability in the case of a smooth barrier, e.g. at the the point contact. The case of the tunnelling through the Josephson barrier is more complicated since the adiabatic approximation is not valid there. The situation might be closer to the regime of a sharp perturbation that deserves a special consideration.

IV. CONCLUSION

Our simple model helps to understand that, even in a two-particle system, the tunnelling is a complex process that can be noticeably influenced by the finite size of a tunnelling object and by its intrinsic degrees of freedom. We pointed out the necessity to study the behavior of the normal modes of a tunnelling system and its adiabatic polarizability (or deformability) by the barrier potential. The role of restructuring of complex particles in the process of a nuclear reaction was emphasized in a different context in refs. [10,11].

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